THE NCNR DISK CHOPPER TIME-OF-FLIGHT SPECTROMETER (DCS)

The recently commissioned Disk Chopper Spectrometer (DCS) is a versatile state-of-the-art instrument that is primarily intended for studies of diffusional processes and low energy excitations in materials. It has no equal in North America and is fully competitive with comparable instruments in Europe.

The spectrometer is shown schematically in Fig. 1. Following a tapered offset guide assembly (“neutron optical filter”) that removes almost all of the γ-rays and high energy neutrons from the reactor beam [1], seven phased disk choppers supply monochromatic bursts of neutrons at the sample position. Three parallel banks of 6 atmosphere ^{3}He detectors, of 400 mm active length, are placed 4010 mm from the sample position, and ≈ 90 % of the space between the sample and the detectors is argon-filled. Each of the 913 rectangular cross section detectors subtends ≈ 0.5° in the scattering plane. The central bank provides continuous angular coverage from -30° to -5° and from 5° to 140°. The overall detector coverage is ≈ 0.65 sr, double that of the IN5 spectrometer at the Institut Laue Langevin, Grenoble. Presently fitted with a ≈ 50 mm long room temperature beryllium filter, the instrument operates at wavelengths greater than ≈ 4.1 Å. The beryllium will shortly be replaced with an assembly of cold oriented graphite, ≈ 100 mm in length, permitting measurements down to ≈ 2.3 Å. (Wavelengths near 3.33 Å and 6.67 Å will be unavailable.) The first two and last two choppers are fitted with three slots of different widths, enabling a choice among three “resolution modes” at a given wavelength and master chopper speed. The neutron current density at the sample and the energy resolution width at the detectors are shown in Figs. 2 and 3 respectively. In designing and building the DCS, great care has been taken to ensure that distances and detector locations are accurately known. The stability of the chopper phasing results in a resolution lineshape with a sharp leading edge. The sample area is easily accessed at beam level and from above. The data acquisition system has been carefully designed and is extremely reliable. We plan to modify it so that crude pulse height spectra can be extracted. The software is user-friendly and will be improved as time permits. Planned improvements, apart from the crystal filter replacement, include removal of the two innermost reflecting plates within the guides after the first chopper; this will increase the flux with little reduction in versatility. With the new cold source and these optics improvements we anticipate a threefold improvement in flux within the next year.

The first officially approved experiment using the DCS was a comparative study [2] of native bovine α-lactalbumin (BLA) and α-lactalbumin in a “molten globular” state (MBLA); the latter state is partially folded and compact, with native-like secondary structure but lacking the side-chain packing that characterizes the native state. Molten globules play an important role in understanding protein folding mechanisms, and molten globules also participate in important cellular functions. The DCS measurements (Fig. 4) confirm and extend previous results [3, and see also the article by Z. Bu et al. on

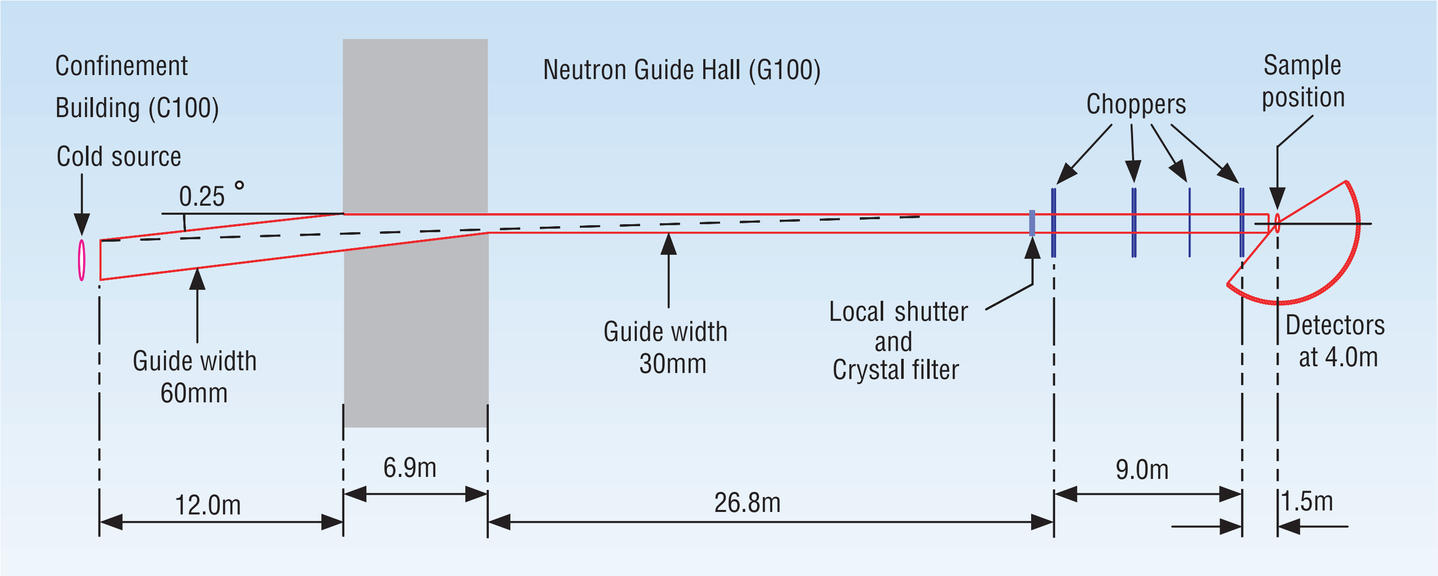

FIGURE 1. A schematic plan view of the DCS.

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p. 20 of this report] obtained with the Fermi chopper spectrometer (FCS); the improved energy resolution of the DCS adds confidence to the earlier results, especially for BLA. The structural differences between BLA and MBLA are reflected in the dynamics on time scales of order 10 ps to 100 ps, whereas complementary measurements have shown that the high frequency dynamics are virtually unchanged.

The moniker "boson peak" has of late been associated with an excess feature that shows up in the vibrational density of states of many materials, generally in the Debye region, between 1 meV and 10 meV. While the molecular origin of the peak is unclear, its characteristic energy suggests that it is a collective excitation between the low energy acoustic modes and localized high energy optic modes (representing local bond vibrations, librations, bendings, etc.). In a recent experiment [4] the thermal softening of the boson peak was studied in detail in a polyester carbonate copolymer that had already been extensively studied using the FCS and the NCNR backscattering spectrometer. The DCS is particularly well suited for such a study because of the large solid angle of detectors and the large beam size. The analysis of the data is in progress.

Other materials recently studied using the DCS include carbon nanotubes and superionic proton conductors.

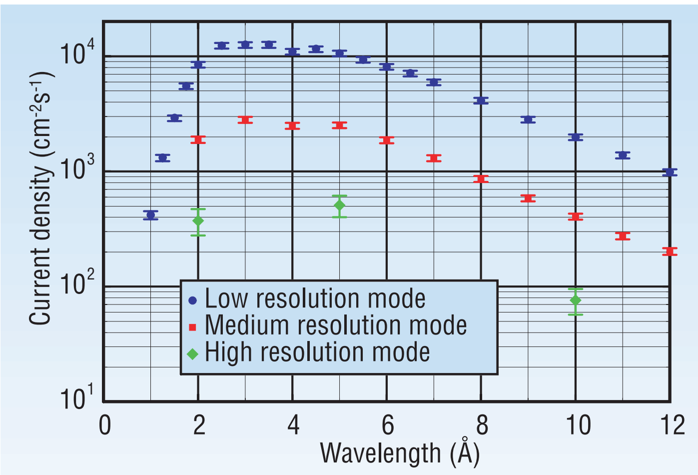

FIGURE 2. The neutron current density at the sample position with all choppers spinning at 20 000 rpm. Measured values are shown for the three "resolution modes" of the instrument.

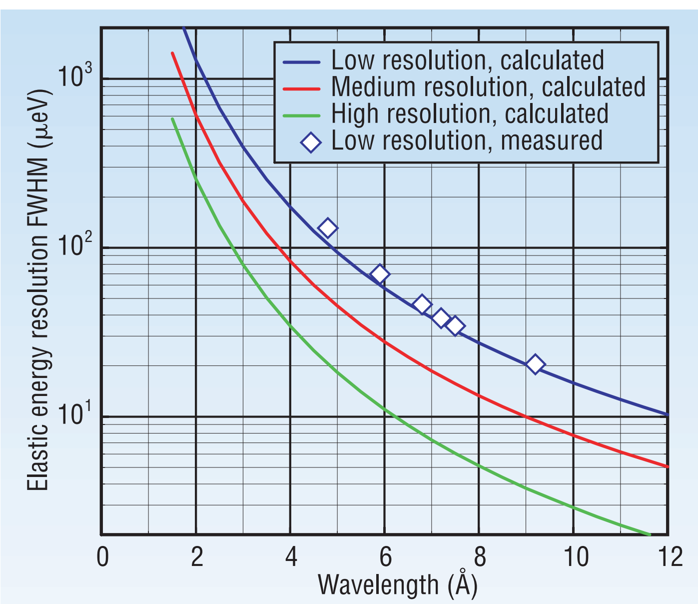

FIGURE 3. Calculated resolution widths (full widths at half maximum height) for the three "resolution modes" of the instrument. Some experimental widths are also shown.

REFERENCES

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[3] Z. Bu, D. A. Neumann, S.-H. Lee, C. M. Brown, D. M. Engelman, and C. C. Han, J. Mol. Biol. **301**, 525 (2000).

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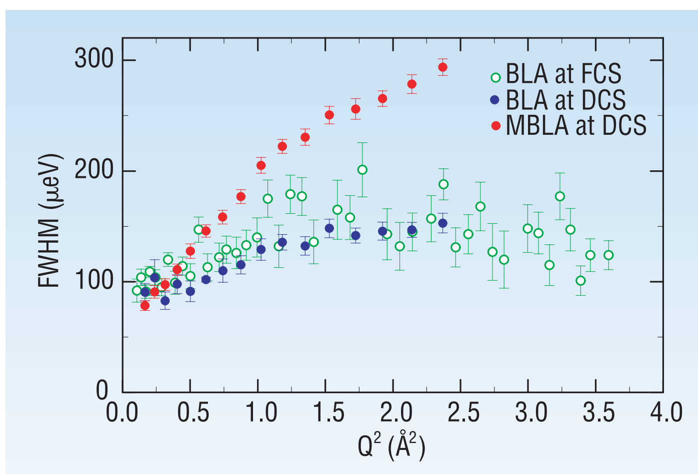

FIGURE 4. The Q dependence of the full-width at half maximum height of the quasielastic Lorentzian peak for native bovine α-lactalbumin (BLA) and for molten globular bovine α-lactalbumin (MBLA) in 8M urea [2]. Results [3] for BLA from the Fermi chopper spectrometer (FCS) are shown for comparison.